Süleyman Demirel Üniversitesi
Fen Bilimleri Enstitüsü Dergisi
Cilt 22, Özel Sayı, 285-289, 2018

Süleyman Demirel University
Journal of Natural and Applied Sciences
Volume 22, Special Issue, 285-289, 2018

DOI: 10.19113/sdufbed.61724

The Values of Eccentricity-Based Topological Indices of Diamond Graphs

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(Alınış / Received: 01.03.2018, Kabul / Accepted: 25.06.2018, Online Yayınlanma / Published Online: 16.08.2018

Keywords
Graph theory,
Vulnerability,
Eccentricity,
Topological indices,
Diamond graphs

Abstract: Graph theory has been studied different areas such as information, mathematics and chemistry sciences. Especially, it has been the most important mathematical tools for the study the analysis of chemistry. A topological index has been a numerical descriptor of the molecular structure derived from the corresponding molecular graph, also it has used vulnerability of chemical graphs. The vulnerability of a graph has been the reliability of the graph after the disruption of some vertices or edges until breakdown. There are a lot of topological indices which have been defined. Furthermore, the diamond graphs have been defined recently. In this paper, exact formulas for the eccentricity-based topological indices of diamond graphs have been obtained.

Elmas Grafların Dışmerkezliğe Dayalı Topolojiksel İndekslerinin Değerleri

Anahtar Kelimeler
Graf teori,
Zedelenebilirlik,
Dışmerkezlik,
Topolojiksel indeksler,
Elmas graflar

Özet: Graf teori bilgi, matematik ve kimya gibi bilim alanlarında çalışılmaktadır. Özellikle, kimyasal analiz çalışmaları için en önemli matematiksel araçlardan biridir. Bir topolojik indeks, moleküler yapıdan türetilen bir grafın sayısal tanımlayıcısıdır, ayrıca kimyasal grafların zedelenebilirliği için kullanılır. Bir grafın zedelenebilirliği, grafın bazı tepelerinin ve ayrıtlarının zarar görmesinden sonra grafın dayanıklılığıdır. Tanımlanan bir çok topolojiksel indeks vardır. Bununla beraber, son zamanlarda elmas graflar tanımlanmıştır. Bu çalışmada, elmas grafların dışmerkezliğe dayalı topolojiksel indeksleri için tam sonuçlar elde edilmiştir.

1. Introduction

Graph theory's diverse applications in natural science (Chemistry, Biology), especially it is becoming an important component of the mathematical chemistry sciences. In chemical graph theory, a lot of graphical invariants have been used for obtaining correlations of chemical structures with various chemical reactivity, physical properties, or biological activity [1]. These graphical invariants are called topological indices of graphs in this field. There is a large family of distance or degree based topological indices of graphs in chemical graph theory. Also, we can say that the topological indices have been numerical parameters of a graph that are invariant under graph isomorphism. Research on the topological indices have been intensively rising recently. Topological indices have been the numerical indices based on the topology of the atoms and their bonds [1, 2]. There are more than one hundred topological indices. They have characterized the physicochemical properties of the most of molecules. Molecules and molecular compounds are represented by graphs, where their atom types are called by vertices and also their bonds called by edges [3]. Furthermore, the topological indices also compute the vulnerability of a molecular graph same as the network vulnerability parameters [4].

Let $G=(V(G),E(G))$ be a graph of order n and size m, where $n=|V(G)|$ and $m=|E(G)|$. Now, we will give some definitions that we need throughout this paper. For $v\in V(G)$, *the open neighborhood of* v is defined by $N_G(v)=\{u\in V(G)|uv\in E(G)\}$ and also *closed neighborhood of* v is defined by $N_G[v]=N_G(v)\cup\{v\}$. The *degree of vertex* v in G is the number of edges incident to v, also it is the size of its open neighborhood, and denoted by $deg_G(v)$ [5]. Let u and v be any two vertices. The distance between u and v in the graph G is the length of a shortest path between them, also is denoted by $d_G(u,v)$. The diameter $diam(G)$ of a graph G is defined the length of largest path which is the shortest path between any two vertices of G. The *eccentricity value* of vertex u in G denoted by $\varepsilon_G(u)$, that is the length of largest path between a vertex u and any other *vertex* v of G,

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$\varepsilon_G(u) = max_{v\in V(G)} d_G(u,v)$ [6]. Let $f = uv$ be an edge in $E(G)$. Then, the *degree* of the edge *f*, denoted by $deg_G(f)$, is defined to be

$$deg_G(f) = deg_G(u) + deg_G(v) - 2.$$

Let $f_1 = u_1v_1$ and $f_2 = u_2v_2$ be two edges in $E(G)$. The *distance* between f_1 and f_2, denoted by $d_G(f_1,f_2)$, is defined to:

$$d_G(f_1,f_2) = min\{d_G(u_1,u_2), d_G(u_1,v_2), d_G(v_1,u_2), d_G(v_1,v_2)\}.$$

The *eccentricity value* of edge *f* in *G*, denoted by $\varepsilon_G(f)$ is defined as:

$$\varepsilon_G(f) = max\{d_G(f,e) | e \in E(G)\} \text{ [6]}.$$

Let $L_n \cong P_n \square P_2, n \geq 2$, be ladder with the vertex set $V(L_n) = \{v_i, u_i : i = 1,2,\dots,n\}$. Then, the edge set $E(L_n) = \{v_iv_{i+1}, u_iu_{i+1} : i = 1,2,\dots,n-1\} \cup \{v_iu_i : i = 1,2,\dots,n\}$, see [7]. If we add the edges $u_iv_{i+1}, i = 1,2,\dots,n-1$, to the ladder L_n and remove the vertex u_n with both incident edges $u_{n-1}u_n$ and u_nv_n, then a triangular ladder TL_n is obtained. A diamond graph $Br_n, n \geq 3$, is obtained by joining a single vertex w to all vertices $v_i, i = 1,2,\dots,n$, of a triangular ladder TL_n [8, 9]. The vertex set of Br_n is $V(Br_n) = \{w\} \cup \{v_i : i = 1,2,\dots,n\} \cup \{u_i : i = 1,2,\dots,n-1$ and the edge set is as follows:

$$\begin{aligned} E(Br_n) = &\{u_iu_{i+1} : i = 1,2,\dots,n-2\} \\ &\cup \{v_iv_{i+1} : i = 1,2,\dots,n-1\} \\ &\cup \{u_iv_i : i = 1,2,\dots,n-1\} \\ &\cup \{u_iv_{i+1} : i = 1,2,\dots,n-1\} \\ &\cup \{wv_i : i = 1,2,\dots,n\}. \end{aligned}$$

Thus, $|V(Br_n)| = 2n$ and $|E(Br_n)| = 5n - 5$ are obtained.

In Figure 1, we display the diamond graphs Br_3 and Br_4, and also the diamond graph Br_5 is shown in Figure 2 .

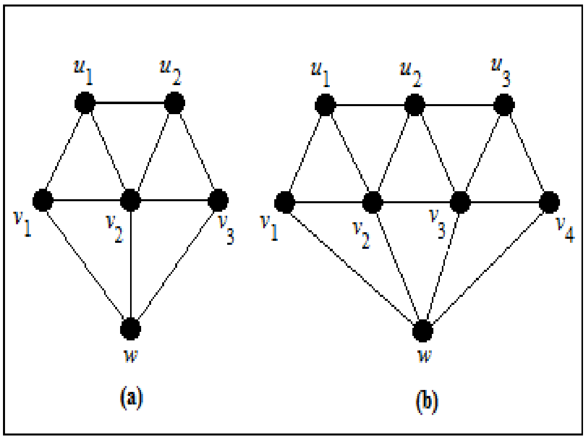

Figure 1. (a) The graph Br_3 **(b)** the graph Br_4

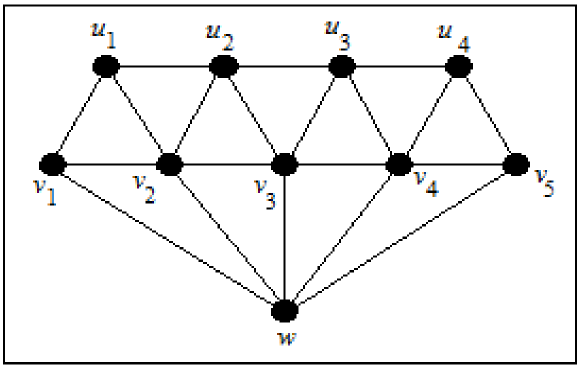

Figure 2. The graph Br_5

First topological index namely Wiener index in chemistry is developed by chemist Harold Wiener [1]. The aim of Wiener index is to the sum of half of the distances between every pair of vertices of G and is defined as:

$$W(G) = \frac{1}{2}\left(\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(v_i, v_j)\right)$$

There are a lot of topological indices were introduced after defined the wiener index, also they divided according to some properties of the graph. One of their most important ones is known that distance of any two vertices (*or atoms*) and edges (*or bonds*). In 2000, Gupta et al. [10] introduced new topological index namely *connective eccentricity* index denoted by $\xi^{ce}(G)$ for the graph *G*. It is defined with as follows:

$$\xi^{ce}(G) = \sum_{u\varepsilon V(G)} (deg_G(u)/\varepsilon_G(u))$$

The eccentric connectivity index $\xi^{c}(G)$ was defined by Sharma et al [11]. The *eccentric connectivity* index is denoted by $\xi^{c}(G)$ for the any graph G , also is defined as follows:

$$\xi^{c}(G) = \sum_{u\varepsilon V(G)} (deg_G(u).\varepsilon_G(u))$$

The first Zagreb index and second Zagreb index of graphs were defined by Gutman et al. [12, 13] . Then the first and second *Zagreb eccentricity* indices $E_1(G)$ and $E_2(G)$ were defined by Vukicevic et al. [14]. The definitions of them are as follows:

$$E_1(G) = \sum_{u\in V(G)} (\varepsilon_G(u))^2$$

and

$$E_2(G) = \sum_{uv\in E(G)} (\varepsilon_G(u).\varepsilon_G(v))$$

In [6], the *average eccentricity* index for the any graph G is defined as follows:

$$avec(G) = \frac{1}{|V(G)|} \sum_{u \in V(G)} \varepsilon_G(u)$$

Recently, a new topological index namely *edge eccentric connectivity index*, has been studied. This new index was defined by Xu et al. [15] and has been studied by some authors [16, 17, 18, 19]. The *edge eccentric connectivity* index of a graph G, denoted by $\xi_e^c(G)$, is defined as follows:

$$\xi_e^c(G) = \sum_{f \in E(G)} \left(deg_G(f).\varepsilon_G(f)\right)$$

where $\varepsilon_G(f)$ is eccentricity value and $deg_G(f)$ is degree of an edge f in the graph G. Each *eccentricity-based* indices have been much used recently in the QSAR/QSPR studies.

In this paper, some eccentricity-based topological indices such as connective eccentricity, eccentric connectivity, Zagreb eccentricity, average eccentricity and edge eccentric connectivity have been computed for the diamond graphs.

2. The Exact Values of Eccentricity-Based Topological Indices of Diamond Graphs

In this chapter, we compute the values of $\xi^{ce}(Br_n)$, $\xi^{c}(Br_n)$, $E_1(Br_n)$, $E_2(Br_n)$, $avec(Br_n)$ and $\xi_e^c(Br_n)$ for the diamond graph of order *2n*. Firstly, we give the degrees of vertices and edges of Br_n . Then, we give a lemma for the diamond graphs.

The degrees of every vertex in the diamond graphs Br_n are as follows:

$deg_{Br_n}(u_1) = deg_{Br_n}(u_{n-1}) = 3$,
$deg_{Br_n}(u_i) = 4$, where $2 \le i \le n-2$,
$deg_{Br_n}(v_1) = deg_{Br_n}(v_n) = 3$,
$deg_{Br_n}(v_i) = 5$, where $2 \le i \le n-1$,
$deg_{Br_n}(w) = n$.

Furthermore, the edges of Br_5 are labeled in Figure 3.

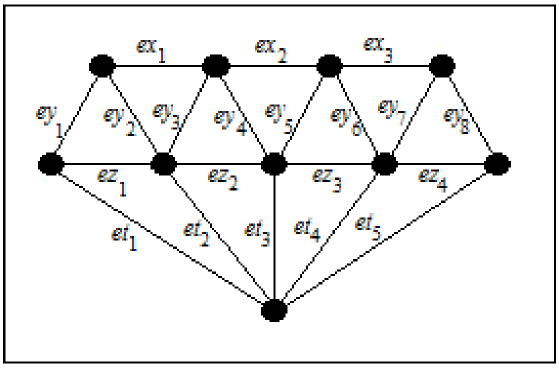

Figure 3. The graph Br_5 whose edges are labeled

The degrees of every edge in the diamond graphs Br_n are as follows:

$deg_{Br_n}(ex_1) = deg_{Br_n}(ex_{n-2}) = 5$,
$deg_{Br_n}(ex_i) = 6$, where $2 \le i \le n-3$,
$deg_{Br_n}(ey_1) = deg_{Br_n}(ey_{2n-2}) = 4$,
$deg_{Br_n}(ey_2) = deg_{Br_n}(ey_{2n-3}) = 6$,
$deg_{Br_n}(ey_i) = 7$, where $3 \le i \le 2n-4$,
$deg_{Br_n}(ez_1) = deg_{Br_n}(ez_{n-1}) = 6$,
$deg_{Br_n}(ez_i) = 8$, where $2 \le i \le n-2$,
$deg_{Br_n}(et_1) = deg_{Br_n}(et_n) = n+1$,
$deg_{Br_n}(et_i) = n+3$, where $2 \le i \le n-1$.

Lemma 2.1. *Let Br_n be a diamond graph of order 2n. If $n \ge 6$, then $diam(Br_n) = 4$.*

Proof. Let $V(Br_n) = V_1(Br_n) \cup V_2(Br_n) \cup \{w\}$, where $V_1(Br_n) = \{u_1, u_2, \dots, u_{n-1}\}$ and $V_2(Br_n) = \{v_1, v_2, \dots, v_n\}$. These vertices can be seen in Figures 1 and 2. Firstly, we consider the vertex w. Clearly, $d_{Br_n}(u_i, w) = 2$ and $d_{Br_n}(v_i, w) = 1$ for each vertex $u_i \in V_1(Br_n)$ and $v_i \in V_2(Br_n)$, respectively. Then, we consider any two vertices as like $u_i \in V_1(Br_n)$ and $v_i \in V_2(Br_n)$. So, we have $d_{Br_n}(u_i, v_x) \le 4$ and $d_{Br_n}(u_i, v_y) \le 3$, where $v_x \in V_1(Br_n) - \{u_i\}$ and $v_y \in V_2(Br_n)$. Similarly, we have $d_{Br_n}(v_i, v_z) \le 2$, where $v_z \in V_2(Br_n) - \{v_i\}$. Then, it is easy to see that $d_{Br_n}(u_i, u_{n-1}) = 4$. Because, a path with 4-length such as $u_1, N_{Br_n}(u_1), w, N_{Br_n}(u_{n-1}), u_{n-1}$, where $N_{Br_n}(u_1)$, $N_{Br_n}(u_{n-1}) \in V_2(Br_n)$ can be found every time for $n \ge 6$. So, we get $diam(Br_n) = 4$. ■

Theorem 2.1 *Let Br_n be a diamond graph of order 2n. If $n \ge 9$, then $\xi^{ce}(Br_n) = \frac{19n-17}{6}$.*

Proof. Finding the eccentricity values of every vertex of Br_n is very similar to Lemma 2.1. Due to $n \ge 9$, the eccentricity values of every vertex in the diamond graphs Br_n are as follows:

$\varepsilon_{Br_n}(u_i) = 4$, where $1 \le i \le n-1$,
$\varepsilon_{Br_n}(v_i) = 3$, where $1 \le i \le n$,
$\varepsilon_{Br_n}(w) = 2$.

Then we get the following:

$$\xi^{ce}(Br_n) = \sum_{u \in V(Br_n)} \left(\frac{deg_{Br_n}(u)}{\varepsilon_{Br_n}(u)}\right)$$

$$= \sum_{i=1}^{n-1} \left(\frac{deg_{Br_n}(u_i)}{\varepsilon_{Br_n}(u_i)}\right) + \sum_{i=1}^{n} \left(\frac{deg_{Br_n}(v_i)}{\varepsilon_{Br_n}(v_i)}\right) + \left(\frac{deg_{Br_n}(w)}{\varepsilon_{Br_n}(w)}\right)$$

$$= \left(\frac{2.3 + (n-3).4}{4}\right) + \left(\frac{2.3 + (n-3).5}{3}\right) + \left(\frac{n}{2}\right)$$

$$= \frac{19n-17}{6}. \quad ■$$

Theorem 2.2. *Let Br_n be a diamond graph of order 2n. If $n \geq 9$, then $\xi^c(Br_n) = 33n - 36$.*

Proof. The degree and eccentricity values of every vertex of Br_n are found in the Theorem 2.1.
Thus, we have

$$\xi^c(Br_n) = \sum_{u \varepsilon V(Br_n)} \left(deg_{Br_n}(u).\varepsilon_{Br_n}(u) \right)$$

$$= \sum_{i=1}^{n-1} \left(deg_{Br_n}(u_i).\varepsilon_{Br_n}(u_i) \right) + \sum_{i=1}^{n} \left(deg_{Br_n}(v_i).\varepsilon_{Br_n}(v_i) \right) + \left(deg_{Br_n}(w).\varepsilon_{Br_n}(w) \right)$$

$$= \left(2.(3.4) + (n-3).(4.4)\right) + \left(2.(3.3) + (n-2).(5.3)\right) + 2n$$

$$= 33n - 36. \quad \blacksquare$$

Theorem 2.3. *Let Br_n be a diamond graph of order 2n. If $n \geq 9$, then $E_1(Br_n) = 25n - 12$ and also if $n \geq 12$, then $E_2(Br_n) = 55n - 65$.*

Proof. The degrees and eccentricity values of every vertex of Br_n are found in the Theorem 2.1.

Thus, we have

$$E_1(Br_n) = \sum_{u \in V(Br_n)} \left(\varepsilon_{Br_n}(u) \right)^2$$

$$= \sum_{i=1}^{n-1} (\varepsilon_{Br_n}(u_i))^2 + \sum_{i=1}^{n} (\varepsilon_{Br_n}(v_i))^2 + (\varepsilon_{Br_n}(w))^2$$

$$= \left((\mathrm{n}-1).4^2\right) + (\mathrm{n}.3^2) + 2^2$$

$$= 25n - 12. \quad \blacksquare$$

Clearly, in the graph Br_n the numbers of edges ex_i, ey_i, ez_i and et_i are $n-2$, $2n-2$, $n-1$ and n, respectively.

Thus, we have

$$E_2(Br_n) = \sum_{uv \in E(Br_n)} \left(\varepsilon_{Br_n}(u).\varepsilon_{Br_n}(v) \right)$$

$$= \sum_{i=1}^{n-2} \left(\varepsilon_{Br_n}(u).\varepsilon_{Br_n}(u) \right) + \sum_{i=1}^{2n-2} \left(\varepsilon_{Br_n}(u).\varepsilon_{Br_n}(v) \right) + \sum_{i=1}^{n-1} \left(\varepsilon_{Br_n}(v).\varepsilon_{Br_n}(v) \right) + \sum_{i=1}^{n} \left(\varepsilon_{Br_n}(v).\varepsilon_{Br_n}(w) \right)$$

$$= \left((n-2).(4.4)\right) + \left((2n-2).(4.3)\right) + \left((n-1).(3.3)\right) + \left(n.(3.2)\right)$$

$$= 55n - 65. \quad \blacksquare$$

Theorem 2.4. *Let Br_n be a diamond graph of order 2n. If $n \geq 9$, then $avec(Br_n) = \frac{7}{2} - \frac{1}{n}$.*

Proof. The degree and eccentricity values of every vertex of Br_n are found in the Theorem 2.1.
Then, we get

$$avec(Br_n) = \frac{1}{|V(Br_n)|} \sum_{u \in V(Br_n)} \varepsilon_{Br_n}(u)$$

$$= \frac{1}{2n} \left(\sum_{i=1}^{n-1} \left(\varepsilon_{Br_n}(u_i) \right) + \sum_{i=1}^{n} \left(\varepsilon_{Br_n}(v_i) \right) + \left(\varepsilon_{Br_n}(w) \right) \right)$$

$$= \frac{1}{2n} \left((n-1).4 + n.3 + 2 \right)$$

$$= \frac{7}{2} - \frac{1}{n}. \quad \blacksquare$$

Theorem 2.5. *Let Br_n be a diamond graph of order 2n. If $n \geq 12$, then $\xi_e^c(Br_n) = 2n^2 + 96n - 166$.*

Proof. The degrees of every edge of Br_n are given at the beginning of the Section 2. For $n \geq 12$, the eccentricity values of every edge of Br_n can be found similar to Theorem 2.1.

Clearly, the eccentricity values of every edge of Br_n are as follows:

$\varepsilon_{Br_n}(ex_i) = 4$, where $1 \leq i \leq n-2$,
$\varepsilon_{Br_n}(ey_i) = 3$, where $1 \leq i \leq 2n-2$,
$\varepsilon_{Br_n}(ez_i) = 3$, where $1 \leq i \leq n-1$,
$\varepsilon_{Br_n}(et_i) = 2$, where $1 \leq i \leq n$.

Thus, we have

$$\xi_e^c(Br_n) = \sum_{f \in E(Br_n)} \left(deg_{Br_n}(f).\varepsilon_{Br_n}(f) \right)$$

$$= \sum_{i=1}^{n-2} \left(deg_{Br_n}(ex_i).\varepsilon_{Br_n}(ex_i) \right) + \sum_{i=1}^{2n-2} \left(deg_{Br_n}(ey_i).\varepsilon_{Br_n}(ey_i) \right) + \sum_{i=1}^{n-1} \left(deg_{Br_n}(ez_i).\varepsilon_{Br_n}(ez_i) \right) + \sum_{i=1}^{n} \left(deg_{Br_n}(et_i).\varepsilon_{Br_n}(et_i) \right)$$

$$= (2.(4.5) + (n-4).(4.6)) + (2.(3.4) + 2.(3.6) + (2n-6).(3.7)) + (2.(3.6) + (n-3).(3.8)) + \left(2.(2.(n+1)) + (n-2).(2.(n+3))\right)$$

$$= 2n^2 + 96n - 166. \quad \blacksquare$$

Next, the vertex eccentricity-based topological indices of diamond graphs for $n \leq 8$ and the edge eccentricity-based topological indices of diamond graphs for $n \leq 11$ are given in Tables 1 and 2, respectively.

Table 1. Some vertex eccentricity-based topological indices of diamond graphs for $n \leq 8$.

	$\xi^{ce}(Br_n)$	$\xi^{c}(Br_n)$	$E_1(Br_n)$	$avec(Br_n)$
$n=3$	25/2	35	21	11/6
$n=4$	13	72	52	5/2
$n=5$	15	110	80	14/5
$n=6$	103/6	150	117	37/12
$n=7$	20	187	149	45/14
$n=8$	137/6	224	181	53/16

Table 2. Some edge eccentricity-based topological indices of diamond graphs for $n \leq 11$.

	$E_2(Br_n)$	$\xi_e^c(Br_n)$
$n=3$	30	50
$n=4$	86	140
$n=5$	151	248
$n=6$	225	382
$n=7$	293	526
$n=8$	361	684
$n=9$	430	842
$n=10$	485	982
$n=11$	540	1126

3. Conclusion

Eccentricity-based topological indices in diamond graphs are considered in this paper while giving an insight of how to evaluate the parameters and derive formulas on diamond graphs. Moreover, we give a lemma for diamond graphs such as diameter of Br_n is 4 for $n \geq 6$.

Acknowledgment

The author is grateful to the area editor and the anonymous referees for their constructive comments and valuable suggestions which have helped me very much to improve the paper.

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